

STRUCTURE SEARCH

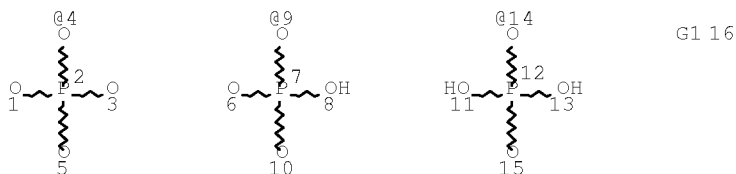
=> d his 150

(FILE 'HCAPLUS' ENTERED AT 11:30:06 ON 13 JUL 2009)

L50 12 S L49 OR L47
 SAV TEMP L50 SAS747HCP/A

=> d que stat 150

L5 STR



VAR G1=4/9/14

NODE ATTRIBUTES:

CONNECT IS X2 RC AT 1
 CONNECT IS X2 RC AT 3
 CONNECT IS E1 RC AT 4
 CONNECT IS E1 RC AT 5
 CONNECT IS X2 RC AT 6
 CONNECT IS E1 RC AT 9
 CONNECT IS E1 RC AT 10
 CONNECT IS E1 RC AT 14
 CONNECT IS E1 RC AT 15

DEFAULT MLEVEL IS ATOM

DEFAULT ECLEVEL IS LIMITED

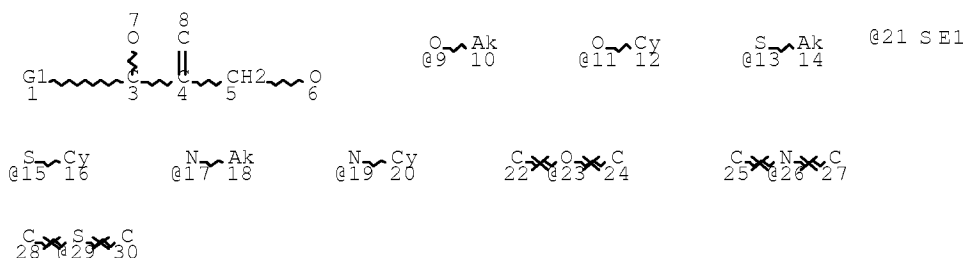
GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED

NUMBER OF NODES IS 16

STEREO ATTRIBUTES: NONE

L8 STR



VAR G1=OH/NH2/21/9/11/13/15/17/19/23/26/29

NODE ATTRIBUTES:

HCOUNT IS E1 AT 21
 CONNECT IS E1 RC AT 7
 DEFAULT MLEVEL IS ATOM
 DEFAULT ECLEVEL IS LIMITED
 ECOUNT IS M1-X18 C AT 10
 ECOUNT IS M1-X18 C AT 14
 ECOUNT IS M1-X18 C AT 18

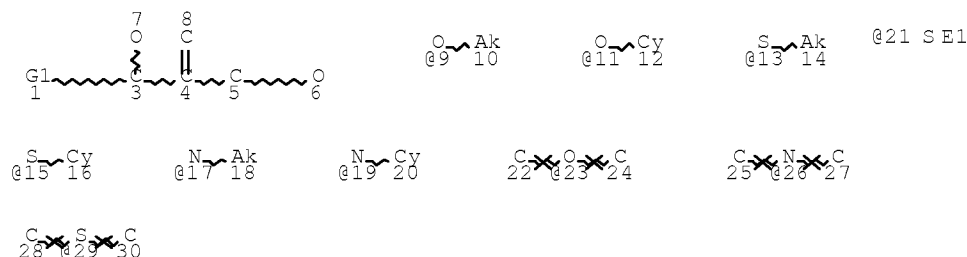
GRAPH ATTRIBUTES:

10/596,747-301496-EIC SEARCH

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L15 257255 SEA FILE=REGISTRY SSS FUL L5
L19 STR



VAR G1=OH/NH2/21/9/11/13/15/17/19/23/26/29

NODE ATTRIBUTES:

HCOUNT IS E1 AT 21
CONNECT IS E1 RC AT 7
DEFAULT MLEVEL IS ATOM
DEFAULT ECLEVEL IS LIMITED
ECOUNT IS M1-X18 C AT 10
ECOUNT IS M1-X18 C AT 14
ECOUNT IS M1-X18 C AT 18

GRAPH ATTRIBUTES:

RING(S) ARE ISOLATED OR EMBEDDED
NUMBER OF NODES IS 29

STEREO ATTRIBUTES: NONE

L22 30 SEA FILE=REGISTRY SUB=L15 SSS FUL L5 AND L19
L24 18 SEA FILE=REGISTRY SUB=L15 SSS FUL L5 AND L8
L25 QUE SPE=ON ABB=ON PLU=ON CH2O OR C2H4O OR C3H6O OR C4C8O
L26 6 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L24 AND L25
L28 2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L24 AND 75-21-8/CRN
L30 0 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L24 AND 75-56-9/CRN
L31 2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L22 AND 75-21-8/CRN
L32 0 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L22 AND 75-56-9/CRN
L38 21108 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON 553.3/RID
L39 2 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L24 AND L38
L40 8 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L26 OR L28 OR (L30 OR L31 OR L32) OR L39
L43 30 SEA FILE=REGISTRY SPE=ON ABB=ON PLU=ON L22 OR L24
L44 QUE SPE=ON ABB=ON PLU=ON PY=<2003 NOT P/DT
L45 QUE SPE=ON ABB=ON PLU=ON (PY=<2003 OR PRY=<2003 OR AY=<2003 OR MY=<2003 OR REVIEW/DT) AND P/DT
L46 17 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L43
L47 12 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L46 AND (L44 OR L45)
L48 3 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L40
L49 1 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L48 AND L47
L50 12 SEA FILE=HCAPLUS SPE=ON ABB=ON PLU=ON L49 OR L47

STRUCTURE SEARCH RESULTS

=> d 150 1-12 ibib ed abs hitstr hitind

L50 ANSWER 1 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2005:568976 HCAPLUS Full-text
 DOCUMENT NUMBER: 143:83603
 TITLE: One-part self-etching, self-priming dental
 adhesive composition
 INVENTOR(S): Klee, Joachim E.; Lehmann, Uwe; Walz, Uwe
 PATENT ASSIGNEE(S): Dentsply Detrey GmbH, Germany
 SOURCE: Eur. Pat. Appl., 30 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: ~~Patent~~
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1548021	A1	20050629	EP 2003-29824	2003 1223
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EP 1548021	B1	20070321		
R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
AT 357450	T	20070415	AT 2003-29824	2003 1223
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CA 2551228	A1	20050714	CA 2004-2551228	2004 1215
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WO 2005063778	A1	20050714	WO 2004-EP14307	2004 1215
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RW: BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM, AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IS, IT, LT, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR, BF, BJ, CF, CG, CI, CM, GA, GN, GQ, GW, ML, MR, NE, SN, TD, TG				
JP 2007520465	T	20070726	JP 2006-545998	2004 1215
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US 20070293642	A1	20071220	US 2007-596747	2007 0508
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PRIORITY APPLN. INFO.:			EP 2003-29824	A 2003 1223
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			WO 2004-EP14307	W

10/596,747-301496-EIC SEARCH

2004

1215

ED Entered STN: 01 Jul 2005

AB One-part self-etching, self-priming dental adhesive composition having a pH of at most 2 comprises (a) a polymerizable acidic phosphoric acid ester monomer; (b) one or more polymerizable acidic monomers; (c) a polymerizable N-substituted alkylacrylic or acrylic acid amide monomer; (d) an organic and/or inorg. acid; (e) an organic water soluble solvent and/or water; and (f) polymerization initiator, inhibitor and stabilizer. An adhesive polymer was prepared from 2-acrylamido-2-methyl-propane-sulfonic acid, 3, (4), 8, (9)-bis(acrylamido methyl) tricyclo-5.2.1.02,6 decane, Et 2-[13-dihydrogen phosphoryl-13,2-dioxatridecyl]acrylate, and N,N'-bisacrylamido-N,N'-diethyl-1,3-propane.

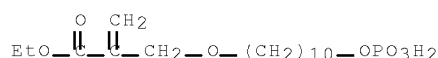
IT 752234-98-3P 752235-00-0P 855894-56-3P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(one-part self-etching, self-priming dental adhesive composition)

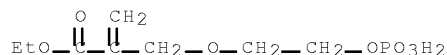
RN 752234-98-3 HCAPLUS

CN 2-Propenoic acid, 2-[[[10-(phosphonooxy)decyl]oxy]methyl]-, 1-ethyl ester (CA INDEX NAME)



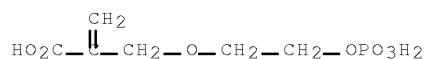
RN 752235-00-0 HCAPLUS

CN 2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]-, 1-ethyl ester (CA INDEX NAME)



RN 855894-56-3 HCAPLUS

CN 2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]- (CA INDEX NAME)



IT 855894-57-4P, 2-Acrylamido-2-methyl-propane-sulfonic acid-3, (4), 8, (9)-bis(acrylamido methyl) tricyclo-5.2.1.02,6 decane-Ethyl 2-[13-dihydrogen

phosphoryl-13,2-dioxatridecyl]acrylate-N,N'-Bisacrylamido-N,N'-diethyl-1,3-propane copolymer 855894-58-5P

RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(one-part self-etching, self-priming dental adhesive composition)

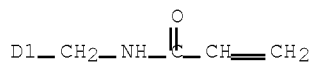
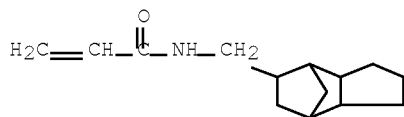
RN 855894-57-4 HCAPLUS

CN 2-Propenoic acid, 2-[[[10-(phosphonooxy)decyl]oxy]methyl]-, 1-ethyl ester, polymer with 2-methyl-2-[(1-oxo-2-propen-1-yl)amino]-1-propanesulfonic acid, N,N'-[[octahydro-4,7-methano-1H-indene-1,5(1,6 or 2,5)diyl]bis(methylene)]bis[2-propenamide] and N,N'-1,3-propanediylbis[N-ethyl-2-propenamide] (CA INDEX NAME)

10/596,747-301496-EIC SEARCH

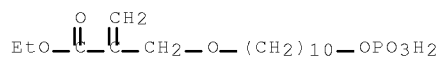
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CRN 855532-00-2
CMF C18 H26 N2 O2
CCI IDS



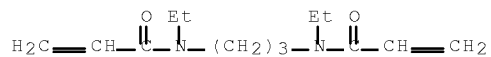
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CRN 752234-98-3
CMF C16 H31 O7 P



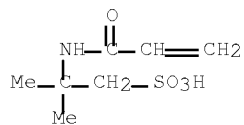
CM 3

CRN 442200-41-1
CMF C13 H22 N2 O2



CM 4

CRN 15214-89-8
CMF C7 H13 N O4 S



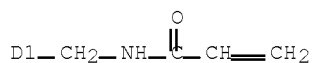
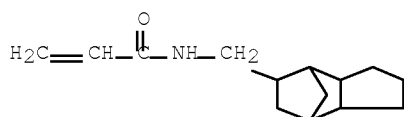
RN 855894-58-5 HCAPLUS
CN 2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy)methyl]-, 1-ethyl ester, polymer with 2-methyl-2-[(1-oxo-2-propenyl)amino]-1-

10/596,747-301496-EIC SEARCH

propanesulfonic acid, N,N-[[octahydro-4,7-methano-1H-indene-1,5(1,6 or 2,5)diyl]bis(methylene)]bis[2-propenamide] and N,N'-1,3-propanediylbis[N-ethyl-2-propenamide] (9CI) (CA INDEX NAME)

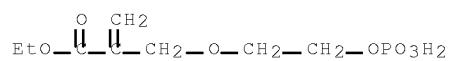
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CRN 855532-00-2
CMF C18 H26 N2 O2
CCI IDS



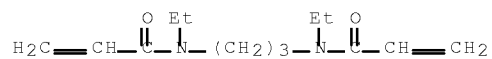
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CRN 752235-00-0
CMF C8 H15 O7 P



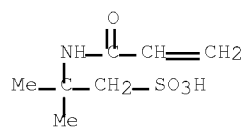
CM 3

CRN 442200-41-1
CMF C13 H22 N2 O2



CM 4

CRN 15214-89-8
CMF C7 H13 N O4 S



10/596,747-301496-EIC SEARCH

IC ICM C07F009-09
ICS C08F030-02; A61K006-00; A61K006-083
CC 63-8 (Pharmaceuticals)
IT 752234-97-2P 752234-98-3P 752234-99-4P
752235-00-0P 855894-56-3P
RL: IMF (Industrial manufacture); RCT (Reactant); PREP
(Preparation); RACT (Reactant or reagent)
(one-part self-etching, self-priming dental adhesive composition)
IT 855894-57-4P, 2-Acrylamido-2-methyl-propane-sulfonic
acid-3, (4), 8, (9)-bis(acrylamido methyl) tricyclo-5.2.1.02, 6
decane-Ethyl 2-[13-dihydrogen
phosphoryl-13,2-dioxatridecyl]acrylate-N,N'-Bisacrylamido-N,N'-
diethyl-1,3-propane copolymer 855894-58-5P
RL: IMF (Industrial manufacture); THU (Therapeutic use); BIOL
(Biological study); PREP (Preparation); USES (Uses)
(one-part self-etching, self-priming dental adhesive composition)
REFERENCE COUNT: 5 THERE ARE 5 CITED REFERENCES AVAILABLE
FOR THIS RECORD. ALL CITATIONS AVAILABLE
IN THE RE FORMAT

L50 ANSWER 2 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 2005:182218 HCAPLUS Full-text
DOCUMENT NUMBER: 142:287808
TITLE: Lithographic printing plate precursor for
direct imaging from a digital data and
developing in a printing machine without
passing through a development step
INVENTOR(S): Yamasaki, Sumiaki; Makino, Naonori; Inno,
Toshifumi
PATENT ASSIGNEE(S): Fuji Photo Film Co., Ltd., Japan
SOURCE: U.S. Pat. Appl. Publ., 50 pp.
CODEN: USXXCO
DOCUMENT TYPE: ~~Patent~~
LANGUAGE: English
FAMILY ACC. NUM. COUNT: 1
PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
US 20050048398	A1	20050303	US 2004-896070	2004 0722
US 7183038	B2	20070227		
EP 1500498	A2	20050126	EP 2004-17306	2004 0722
EP 1500498	A3	20051012		
R: AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR, HU, IE, IT, LI, LU, MC, NL, PL, PT, RO, SE, SI, SK, TR				
JP 2005238816	A	20050908	JP 2004-214190	2004 0722
PRIORITY APPLN. INFO.:				
			JP 2003-277448	A 2003 0722
			JP 2004-652	A 2004 0105
			JP 2004-17599	A

10/596,747-301496-EIC SEARCH

2004
0126

JP 2004-214190 A

2004
0722

OTHER SOURCE(S): MARPAT 142:287808

ED Entered STN: 04 Mar 2005

AB A lithog. printing plate precursor is described for recording an image directly from a digital data and development in a printing machine without passing through a development step. The precursor provides lithog. printing plates with improved press life and stain resistance. Thus, the precursor coating composition comprises an image-forming layer containing a polymerization initiator and a polymerizable compound, and a hydrophilic support. The composition includes a compound containing at least one functional group interacting with a surface of the hydrophilic support. This compound is one of a phosphonic acid and a phosphoric acid amide.

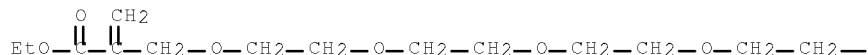
IT 847226-71-5

RL: TEM (Technical or engineered material use); USES (Uses)
(lithog. printing plate precursor for direct imaging from
digital data and in-press development)

RN 847226-71-5 HCAPLUS

CN 2-Propenoic acid, 2-(15,15-dihydroxy-15-oxido-2,5,8,11,14-pentaoxa-
15-phosphapentadec-1-yl)-, 1-ethyl ester (CA INDEX NAME)

PAGE 1-A



PAGE 1-B

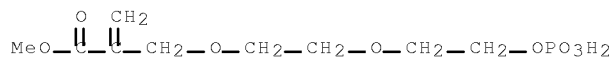


IT 847204-83-5 847204-84-6

RL: TEM (Technical or engineered material use); USES (Uses)
(phosphonic derivative; lithog. printing plate precursor for direct
imaging from digital data and in-press development)

RN 847204-83-5 HCAPLUS

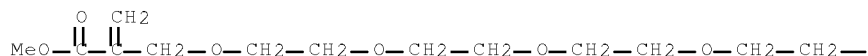
CN 2-Propenoic acid, 2-(9,9-dihydroxy-9-oxido-2,5,8-trioxa-9-
phosphanon-1-yl)-, 1-methyl ester (CA INDEX NAME)



RN 847204-84-6 HCAPLUS

CN 2-Propenoic acid, 2-(15,15-dihydroxy-15-oxido-2,5,8,11,14-pentaoxa-
15-phosphapentadec-1-yl)-, 1-methyl ester (CA INDEX NAME)

PAGE 1-A



10/596,747-301496-EIC SEARCH

PAGE 1-B

— OPO3H2

IC ICM G03C001-492
 INCL 430270100
 CC 74-5 (Radiation Chemistry, Photochemistry, and Photographic and
 Other Reprographic Processes)
 IT 847204-87-9 847204-88-0 847204-89-1 847204-90-4
 847204-91-5 847226-71-5
 RL: TEM (Technical or engineered material use); USES (Uses)
 (lithog. printing plate precursor for direct imaging from
 digital data and in-press development)
 IT 80730-17-2 223681-84-3 847204-73-3 847204-74-4 847204-75-5
 847204-76-6 847204-77-7 847204-78-8 847204-82-4
 847204-83-5 847204-84-6 847204-85-7
 847232-64-8
 RL: TEM (Technical or engineered material use); USES (Uses)
 (phosphonic derivative; lithog. printing plate precursor for direct
 imaging from digital data and in-press development)
 REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L50 ANSWER 3 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2004:732258 HCAPLUS Full-text
 DOCUMENT NUMBER: 141:243056
 TITLE: Polymerizable phosphoric acid ester
 derivatives for dental compositions
 INVENTOR(S): Klee, Joachim E.; Lehmann, Uwe; Walz, Uwe;
 Liu, Huaibing
 PATENT ASSIGNEE(S): Dentsply Detrey GmbH, Germany
 SOURCE: Eur. Pat. Appl., 20 pp.
 CODEN: EPXXDW
 DOCUMENT TYPE: Patent
 LANGUAGE: English
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
EP 1454911	A1	20040908	EP 2003-5174	2003 0307

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R: AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, SK				
CA 2518202	A1	20040916	CA 2004-2518202	2004 0305

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WO 2004078100	A2	20040916	WO 2004-EP2289	2004 0305
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WO 2004078100	A3	20041028		
W: AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ,				

10/596,747-301496-EIC SEARCH

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 ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP,
 KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD,
 MG, MK, MN, MW, MX, MZ, NA, NI
 RW: BW, GH, GM, KE, LS, MW, MZ, SD, SL, SZ, TZ, UG, ZM, ZW,
 AT, BE, BG, CH, CY, CZ, DE, DK, EE, ES, FI, FR, GB, GR,
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 EP 1601679 A2 20051207 EP 2004-717576

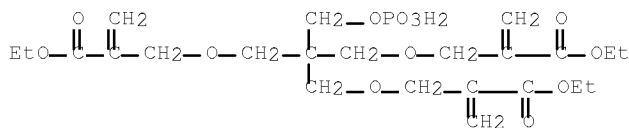
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 JP 2006520344 T 20060907 JP 2006-504563
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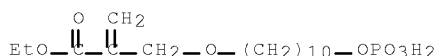
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 US 20060246017 A1 20061102 US 2006-548362
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 0626

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 PRIORITY APPLN. INFO.: EP 2003-5174 A
 2003
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 WO 2004-EP2289 W
 2004
 0305

ED Entered STN: 09 Sep 2004
 AB The present invention provides a polymerizable phosphoric acid ester derivative for use
 in dental compns. E.g., 2,2,2-tris(2,6-dioxa-4-methylene-5-oxo-octyl)ethanol
 phosphoric acid ester was prepared from pentaerythritol, Et chloromethacrylate, and
 then treatment with the product with POCl3 and hydrolyzed.
 IT 752234-96-1P 752234-98-3P 752235-00-0P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL
 (Biological study); PREP (Preparation); USES (Uses)
 (polymerizable phosphoric acid ester derivs. for dental
 compns.)
 RN 752234-96-1 HCAPLUS
 CN 2-Propenoic acid, 2,2'-[[2-[[[2-(ethoxycarbonyl)-2-
 propenyl]oxy]methyl]-2-[(phosphonooxy)methyl]-1,3-
 propanediyl]bis(oxymethylene)]bis-, 1,1'-diethyl ester (9CI) (CA
 INDEX NAME)

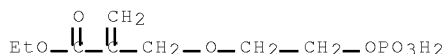


RN 752234-98-3 HCAPLUS
 CN 2-Propenoic acid, 2-[[[10-(phosphonooxy)decyl]oxy]methyl]-,
 1-ethyl ester (CA INDEX NAME)



10/596,747-301496-EIC SEARCH

RN 752235-00-0 HCAPLUS
 CN 2-Propenoic acid, 2-[[2-(phosphonooxy)ethoxy]methyl]-, 1-ethyl
 ester (CA INDEX NAME)



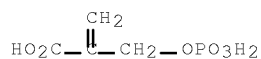
IC ICM C07F009-09
 ICS A61K006-08; C08F030-02
 CC 23-17 (Aliphatic Compounds)
 Section cross-reference(s): 63
 IT 752234-96-1P 752234-98-3P 752235-00-0P
 RL: SPN (Synthetic preparation); THU (Therapeutic use); BIOL
 (Biological study); PREP (Preparation); USES (Uses)
 (polymerizable phosphoric acid ester derivs. for dental
 compns.)
 REFERENCE COUNT: 4 THERE ARE 4 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L50 ANSWER 4 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 2003:69754 HCAPLUS Full-text
 DOCUMENT NUMBER: 139:65615
 TITLE: A fluorescent sensor for
 2,3-bisphosphoglycerate using a europium
 tetra-N-oxide bis-bipyridine complex for both
 binding and signaling purposes
 AUTHOR(S): Best, Michael D.; Anslyn, Eric V.
 CORPORATE SOURCE: The University of Texas at Austin, Austin, TX,
 78712-1167, USA
 SOURCE: Chemistry--A European Journal (2003
), 9(1), 51-57
 CODEN: CEUJED; ISSN: 0947-6539
 PUBLISHER: Wiley-VCH Verlag GmbH & Co. KGaA
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 29 Jan 2003

AB Host 1 was designed and synthesized as a fluorescent sensor for 2,3-bisphosphoglycerate (BPG, 3). The design features a tris-functionalized triethylbenzene core to preorganize binding groups. The three cationic moieties, a tetra-N-oxide bipyridine-europium complex and two ammonium groups, were included to complement the three anionic functionalities on the guest. Beyond acting as a binding site, the europium complex was used to signal binding of the guest through modification of the charge transfer emission. A 1:1 complex with BPG was determined in 50% methanol/acetonitrile with a K_a of $6.7 \times 10^5 \text{ mol}^{-1}$ by monitoring the reduction of the fluorescence signal upon guest addition. In the titration of related glycolytic intermediates lacking a second phosphate (4-6) into host 1, 2:1 host to guest binding was observed. Similarly, control compound 2, which lacks the ammonium groups, binds BPG and 4-6 in a 2:1 fashion. Also, phenylphosphate 7 binds to host 1 in a 1:1 stoichiometry with a K_a over three times less than 3.

IT 549507-60-0
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (fluorescent sensor for 2,3-bisphosphoglycerate using europium
 tetra-N-oxide bis-bipyridine complex for both binding and
 signaling purposes)
 RN 549507-60-0 HCAPLUS
 CN 2-Propenoic acid, 2-[(phosphonooxy)methyl]- (CA INDEX NAME)

10/596,747-301496-EIC SEARCH



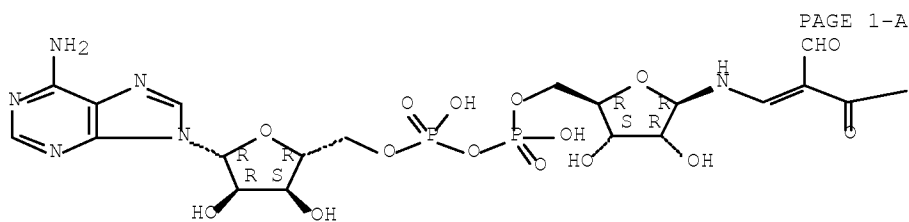
CC 9-5 (Biochemical Methods)
 IT 138-81-8 701-64-4 820-11-1 2553-59-5 ~~549507-60-0~~
 RL: ARU (Analytical role, unclassified); ANST (Analytical study)
 (fluorescent sensor for 2,3-bisphosphoglycerate using europium
 tetra-N-oxide bis-bipyridine complex for both binding and
 signaling purposes)
 REFERENCE COUNT: 59 THERE ARE 59 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L50 ANSWER 5 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1997:118009 HCAPLUS Full-text
 DOCUMENT NUMBER: 126:222078
 ORIGINAL REFERENCE NO.: 126:42871a,42874a
 TITLE: Purification and preliminary characterization
 of
 (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic
 acid synthase, and enzyme involved in
 biosynthesis of the antitumor agent
 sparsomycin
 AUTHOR(S): Parry, Ronald J.; Hoyt, Jeffrey C.
 CORPORATE SOURCE: Dep. of Chemistry, Rice University, Houston,
 TX, 77251, USA
 SOURCE: Journal of Bacteriology (1997),
 179(4), 1385-1392
 CODEN: JOBAA; ISSN: 0021-9193
 PUBLISHER: American Society for Microbiology
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 20 Feb 1997

AB Sparsomycin is an antitumor antibiotic produced by Streptomyces sparsogenes.
 Biosynthetic expts. have previously demonstrated that one component of sparsomycin is
 derived from L-tryptophan via the intermediacy of (E)-3-(4-oxo-6-methyl-5-
 pyrimidinyl)acrylic acid and (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid. An
 enzyme which catalyzes the conversion of (E)-3-(4-oxo-6-methyl-5-pyrimidinyl)acrylic
 acid to (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid was purified 740-fold to
 homogeneity from S. sparsogenes. The mol. mass of the native and denatured enzyme was
 87 kDa, indicating that the native enzyme is monomeric. The enzyme required NAD for
 activity but lacked rigid substrate specificity, since analogs of both inhibited by
 mycophenolic acid. Monovalent cations were required for activity, with potassium ions
 being the most effective. The enzyme exhibited sensitivity toward diethylpyrocarbonate
 and some thiol-directed reagents, and it was irreversibly inhibited by 6-chloropurine.
 The properties of the enzyme suggest it is mechanistically related to inosine-5'-
 monophosphate dehydrogenase.

IT 73435-45-7, NADX
 RL: BPR (Biological process); BSU (Biological study,
 unclassified); BIOL (Biological study); PROC (Process)
 (substrate; purification and preliminary characterization of
 (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid synthase,
 and enzyme involved in biosynthesis of the antitumor agent
 sparsomycin)
 RN 73435-45-7 HCAPLUS
 CN Adenosine 5'-(trihydrogen diphosphate), P'→5'-ester with
 2-formyl-3-(β-D-ribofuranosylamino)-2-propenamide (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



PAGE 1-B

NH₂

CC 7-2 (Enzymes)
 IT 53-84-9, β -NAD 68-94-0, Hypoxanthine 4562-27-0,
 4-Hydroxypyrimidine 7298-93-3, α -NAD 28277-67-0, Uracil
 acrylic acid 73435-45-7, NADX
 RL: BPR (Biological process); BSU (Biological study,
 unclassified); BIOL (Biological study); PROC (Process)
 (substrate; purification and preliminary characterization of
 (E)-3-(2,4-dioxo-6-methyl-5-pyrimidinyl)acrylic acid synthase,
 and enzyme involved in biosynthesis of the antitumor agent
 sparsomycin)
 REFERENCE COUNT: 36 THERE ARE 36 CITED REFERENCES AVAILABLE
 FOR THIS RECORD. ALL CITATIONS AVAILABLE
 IN THE RE FORMAT

L50 ANSWER 6 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1996:684772 HCAPLUS Full-text
 DOCUMENT NUMBER: 125:303429
 ORIGINAL REFERENCE NO.: 125:56755a,56758a
 TITLE: Phosphoric acid esters and their manufacture,
 and polymers from them
 INVENTOR(S): Nagano, Hideaki; Yurugi, Keiji; Nakagawa,
 Koichi; Kita, Juichi
 PATENT ASSIGNEE(S): Nippon Catalytic Chem Ind, Japan
 SOURCE: Jpn. Kokai Tokkyo Koho, 11 pp.
 CODEN: JKXXAF
 DOCUMENT TYPE: ~~Patent~~
 LANGUAGE: Japanese
 FAMILY ACC. NUM. COUNT: 1
 PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 08231564	A	19960910	JP 1995-40604	1995 0228
<--				
PRIORITY APPLN. INFO.:			JP 1995-40604	1995 0228
<--				

OTHER SOURCE(S): MARPAT 125:303429
 ED Entered STN: 20 Nov 1996
 AB Polymers [number-average mol. weight (Mn) 1000-1,000,000] having units
 CH₂CXCHR1OP(O)(OH)₂ and/or CH₂CXCHR1OP(O)(OH)OCHR1CXCH₂, useful for coatings with

10/596,747-301496-EIC SEARCH

excellent adhesion, etc., are obtained from $[\text{CH}_2:\text{CXCHR}_1\text{O}]_n\text{P}(\text{O})(\text{OH})_3-n$, which are manufactured from P compds. and $\text{CH}_2:\text{CXCHR}_1\text{OH}$ ($\text{R}_1 = \text{H}$, organic residues; $\text{X} = \text{CN}$, COR_2 , CO_2R_2 ; $\text{R}_2 = \text{organic residues}$; $n = 1-2$). Thus, 39 g Et α -hydroxymethyl acrylate was treated with 21.3 g P_2O_5 at 50° for 4 h in the presence of hydroquinone monomethyl ether, hydrolyzed, and polymerized at 80° in the presence of 2,2'-azobisisobutyronitrile to give a polymer (M_n 45,000). Then, 25 g polymer was blended with 25 g 1,6-hexanediol diacrylate, 3 g Irgacure 651, and 50 g urethane acrylate manufactured from isophorone diisocyanate 2, triethylene glycol 1, and 2-hydroxyethyl acrylate 2 mols, applied on a steel plate, and cured by irradiation of UV to show cross-cut adhesion 100/100.

IT 183175-03-3P 183175-04-4P

RL: IMF (Industrial manufacture); MOA (Modifier or additive use);

TEM (Technical or engineered material use); PREP (Preparation);

USES (Uses)

(manufacture of allyl alc. phosphoric acid ester polymers for coatings with good adhesion)

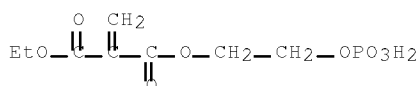
RN 183175-03-3 HCAPLUS

CN Propanedioic acid, methylene-, ethyl 2-(phosphonooxy)ethyl ester, homopolymer (9CI) (CA INDEX NAME)

CM 1

CRN 183175-01-1

CMF C8 H13 O8 P



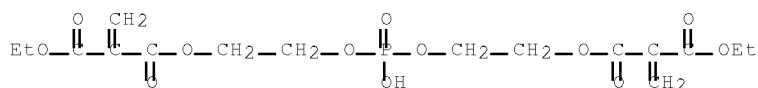
RN 183175-04-4 HCAPLUS

CN 4,7,9,12-Tetraoxa-8-phosphapentadecanedioic acid, 8-hydroxy-2,14-bis(methylene)-3,13-dioxo-, diethyl ester, 8-oxide, polymer with ethenylbenzene (9CI) (CA INDEX NAME)

CM 1

CRN 183175-02-2

CMF C16 H23 O12 P



CM 2

CRN 100-42-5

CMF C8 H8



IT 183175-01-1P 183175-02-2P

RL: IMF (Industrial manufacture); RCT (Reactant); PREP

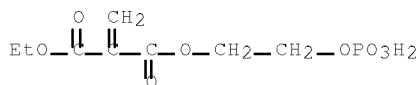
10/596,747-301496-EIC SEARCH

(Preparation); RACT (Reactant or reagent)

(manufacture of allyl alc. phosphoric acid ester polymers for coatings with good adhesion)

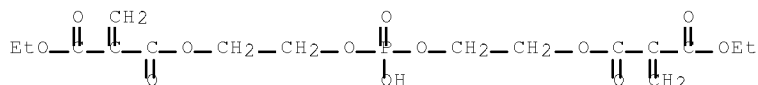
RN 183175-01-1 HCAPLUS

CN Propanedioic acid, 2-methylene-, 1-ethyl 3-[2-(phosphonoxy)ethyl] ester (CA INDEX NAME)



RN 183175-02-2 HCAPLUS

CN 4,7,9,12-Tetraoxa-8-phosphapentadecanedioic acid, 8-hydroxy-2,14-bis(methylene)-3,13-dioxo-, diethyl ester, 8-oxide (9CI) (CA INDEX NAME)



IC ICM C07F009-09

ICS C08F030-02

ICA C09D007-12

CC 42-10 (Coatings, Inks, and Related Products)

Section cross-reference(s): 23, 35

IT ~~183175-03-3P~~ ~~183175-04-4P~~

RL: IMF (Industrial manufacture); MOA (Modifier or additive use); TEM (Technical or engineered material use); PREP (Preparation); USES (Uses)

(manufacture of allyl alc. phosphoric acid ester polymers for coatings with good adhesion)

IT ~~183175-01-1P~~ ~~183175-02-2P~~

RL: IMF (Industrial manufacture); RCT (Reactant); PREP (Preparation); RACT (Reactant or reagent)

(manufacture of allyl alc. phosphoric acid ester polymers for coatings with good adhesion)

L50 ANSWER 7 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1996:368751 HCAPLUS Full-text

DOCUMENT NUMBER: 125:168619

ORIGINAL REFERENCE NO.: 125:31613a,31616a

TITLE: Novel phosphotyrosine mimetics in the design of peptide ligands for pp60src SH2 domain
AUTHOR(S): Shahripour, Aurash; Plummer, Mark S.; Lunney, Elizabeth; Para, Kimberly S.; Stankovic, Charles J.; Rubin, John R.; Humblet, Christine; Fergus, James H.; Marks, James S.; et al.

CORPORATE SOURCE: Dep. Chem., Parke-Davis Pharm. Res., Ann Arbor, MI, 48105, USA

SOURCE: Bioorganic & Medicinal Chemistry Letters (1996), 6(11), 1209-1214
CODEN: BMCLE8; ISSN: 0960-894X

PUBLISHER: Elsevier

DOCUMENT TYPE: Journal

LANGUAGE: English

ED Entered STN: 26 Jun 1996

10/596,747-301496-EIC SEARCH

AB The authors have designed and synthesized a series of phosphorylated penta- and tripeptides of general structures R-Glu-Glu-Ile-Glu-OH and R-Glu-D-Trp-NH₂, where R represents a phosphotyrosine mimetic. These peptides show binding affinity to pp50src SH2 domain in the micromolar range. Data are presented that provide an account of their structure-activity relationships and specificity properties.

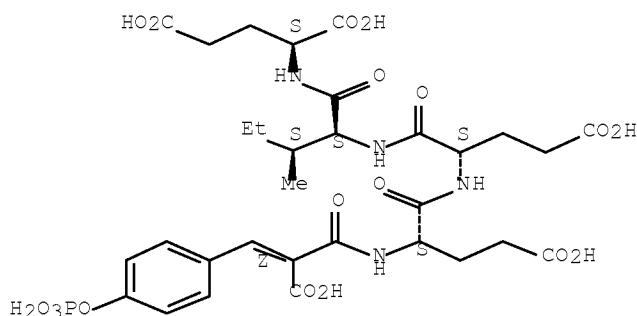
IT 179984-94-2P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of novel phosphotyrosine mimetics in the design of peptide ligands for pp60src SH2 domain)

RN 179984-94-2 HCAPLUS

CN L-Glutamic acid, N-[N-[N-[N-[2-carboxy-1-oxo-3-[4-(phosphonooxy)phenyl]-2-propenyl]-L- α -glutamyl]-L- α -glutamyl]-L-isoleucyl]-, (Z)- (9CI) (CA INDEX NAME)

Absolute stereochemistry.
Double bond geometry as shown.



CC 34-3 (Amino Acids, Peptides, and Proteins)
Section cross-reference(s): 1, 7

IT 159439-02-8P 179984-84-0P 179984-85-1P 179984-86-2P
179984-87-3P 179984-88-4P 179984-89-5P 179984-90-8P
179984-91-9P 179984-92-0P 179984-93-1P 179984-94-2P
179984-96-4P 179984-99-7P 179985-01-4P 179985-03-6P
179985-05-8P 179985-06-9P 179985-08-1P 179985-09-2P
179985-11-6P 180184-68-3P 180184-69-4P 180184-70-7P
180184-71-8P 180184-72-9P 180184-73-0P 180184-74-1P
180184-75-2P 180184-76-3P

RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); SPN (Synthetic preparation); BIOL (Biological study); PREP (Preparation)
(prepn of novel phosphotyrosine mimetics in the design of peptide ligands for pp60src SH2 domain)

L50 ANSWER 8 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN

ACCESSION NUMBER: 1995:603791 HCAPLUS [Full-text](#)

DOCUMENT NUMBER: 123:17973

ORIGINAL REFERENCE NO.: 123:3351a,3354a

TITLE: surface coating of contact lenses

INVENTOR(S): Inomata, Kyoshi; Nakada, Shinji; Koinuma, Yasuyoshi; Nakabayashi, Norio; Ishihara, Kazuhiko

PATENT ASSIGNEE(S): Nippon Oils & Fats Co Ltd, Japan; Nakabayashi Norio

SOURCE: Jpn. Kokai Tokkyo Koho, 9 pp.
CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

10/596,747-301496-EIC SEARCH

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
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JP 07072430	A	19950317	JP 1993-218890	1993 0902

PRIORITY APPLN. INFO.: <--
JP 1993-218890
1993
0902

ED Entered STN: 10 Jun 1995

AB The surface of contact lenses is coated with phospholipid-like vinyl monomers by graft-copolymn. to give surface-coated contact lenses having hydrophilicity, good wettability, and stain-resistance. Thus, γ -methacroyloyloxypropyltris(trimethyloxy)silane, 2,2,2-trifluoroethyl methacrylate, Me methacrylate and ethylene glycol dimethacrylate were reacted and made into contact lenses, which were graft-copolymd. with 2-(methacroyloyloxy)ethyl-2'-(trimethylammonio)ethylphosphate and triethylene glycol dimethacrylate for surface coating.

IT 163674-38-2F

RL: DEV (Device component use); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)
(surface coating of contact lenses)

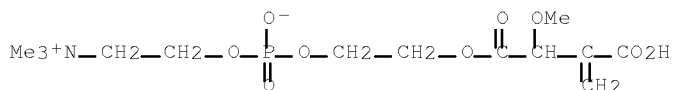
RN 163674-38-2 HCAPLUS

CN 2,5,8,10-Tetraoxa-9-phosphadodecan-12-aminium, 3-(1-carboxyethenyl)-9-hydroxy-N,N,N-trimethyl-4-oxo-, inner salt, 9-oxide, polymer with 1,2-ethanediyl bis(2-methyl-2-propenoate), 1,2-ethanediylbis(oxy-2,1-ethanediyl) bis(2-methyl-2-propenoate), methyl 2-methyl-2-propenoate, 2,2,2-trifluoroethyl 2-methyl-2-propenoate and 3-[3,3,3-trimethyl-1,1-bis[(trimethylsilyl)oxy]disiloxanyl]propyl 2-methyl-2-propenoate (9CI) (CA INDEX NAME)

CM 1

CRN 163674-37-1

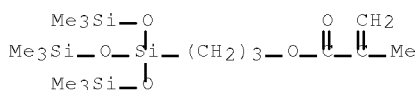
CMF C13 H24 N O9 P



CM 2

CRN 17096-07-0

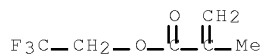
CMF C16 H38 O5 Si4



10/596,747-301496-EIC SEARCH

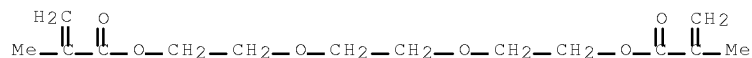
CM 3

CRN 352-87-4
CMF C6 H7 F3 O2



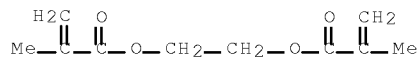
CM 4

CRN 109-16-0
CMF C14 H22 O6



CM 5

CRN 97-90-5
CMF C10 H14 O4



CM 6

CRN 80-62-6
CMF C5 H8 O2



IC ICM G02C007-04
ICS C08F265-06

CC 63-7 (Pharmaceuticals)

Section cross-reference(s): 38

IT 163674-32-6P 163674-34-8P 163674-36-0P ~~163674-38-2P~~
163674-40-6P 163716-64-1P 163716-65-2P

RL: DEV (Device component use); SPN (Synthetic preparation); THU
(Therapeutic use); BIOL (Biological study); PREP (Preparation);
USES (Uses)

(surface coating of contact lenses)

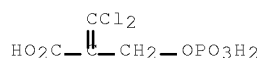
L50 ANSWER 9 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
ACCESSION NUMBER: 1993:4011 HCAPLUS Full-text
DOCUMENT NUMBER: 118:4011

10/596,747-301496-EIC SEARCH

ORIGINAL REFERENCE NO.: 118:851a,854a
 TITLE: Degree of C4 photosynthesis in C4 and C3-C4
 Flaveria species and their hybrids. II.
 Inhibition of apparent photosynthesis by a
 phosphoenolpyruvate carboxylase inhibitor
 AUTHOR(S): Brown, R. Harold; Byrd, George T.; Black,
 Clanton C.
 CORPORATE SOURCE: Dep. Agron., Univ. Georgia, Athens, GA, 30602,
 USA
 SOURCE: Plant Physiology (1983), 100(2),
 947-50
 CODEN: PLPHAY; ISSN: 0032-0889
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 10 Jan 1993

AB Hybrids have been made between species of Flaveria exhibiting varying levels of C4 photosynthesis. The degree of C4 photosynthesis expressed in 4 interspecific hybrids (Flaveria trinervia [C4] + F. linearis [C3-C4], F. brownii [C4-like] + F. linearis, and two three-species hybrids from F. trinervia + [F. brownii + F. linearis]) was estimated by inhibiting phosphoenolpyruvate carboxylase in vivo with 3,3-dichloro-2-dihydroxyphosphinoylmethyl-2-propenoate (DCDP). The inhibitor was fed to detached leaves at a concentration of 4 mM, and apparent photosynthesis was measured at atmospheric levels of CO2 and at 20 and 210 mL L-1 of O2. Photosynthesis at 210 mL L-1 of O2 was inhibited 32% by DCDP in F. linearis, by 60% in F. brownii, and by 87% in F. trinervia. Inhibition in the hybrids ranged from 38 to 52%. The inhibition of photosynthesis by 210 mL L-1 of O2 was increased when DCDP was used, except in the C4 species, F. trinervia, in which photosynthesis was insensitive to O2. Except for F. trinervia, control plants with less O2 sensitivity (more C4-like) exhibited a progressively greater change in O2 inhibition of photosynthesis when treated with DCDP. This increased O2 inhibition probably resulted from decreased CO2 concns. in bundle sheath cells due to inhibition of phosphoenolpyruvate carboxylase. The inhibition of photosynthesis by DCDP is concluded to underestimate the degree of C4 photosynthesis in the interspecific hybrids because increased direct assimilation of atmospheric CO2 by ribulose biphosphate carboxylase may compensate for inhibition of phosphoenolpyruvate carboxylase.

IT 108793-81-3
 RL: BIOL (Biological study)
 (C4 photosynthesis inhibition by, in Flaveria C4 and C3-C4 hybrids)
 RN 108793-81-3 HCAPLUS
 CN 2-Propenoic acid, 3,3-dichloro-2-[(phosphonoxy)methyl]- (CA
 INDEX NAME)

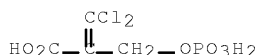


CC 11-6 (Plant Biochemistry)
 IT 108793-81-3
 RL: BIOL (Biological study)
 (C4 photosynthesis inhibition by, in Flaveria C4 and C3-C4 hybrids)

L50 ANSWER 10 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1987:419847 HCAPLUS Full-text
 DOCUMENT NUMBER: 107:19847
 ORIGINAL REFERENCE NO.: 107:3291a,3294a
 TITLE: 3,3-Dichloro-2-dihydroxyphosphinoylmethyl-2-propenoate, a new, specific inhibitor of phosphoenolpyruvate carboxylase
 AUTHOR(S): Jenkins, Colin L. D.; Harris, Roger L. N.; McFadden, Helen G.
 CORPORATE SOURCE: Div. Plant Ind., CSIRO, Canberra, 2601,

10/596,747-301496-EIC SEARCH

Australia
 SOURCE: Biochemistry International (1987),
 14(2), 219-26
 CODEN: BIINDF; ISSN: 0158-5231
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 25 Jul 1987
 AB 3,3-Dichloro-2-dihydroxyphosphinoylmethyl-2-propenoate (I) is a potent linear competitive inhibitor of maize leaf phosphoenolpyruvate carboxylase [$K_i(\text{Mn}^{2+}) = 3 \mu\text{M}$; $K_i(\text{Mg}^{2+}) = 80 \mu\text{M}$]. In contrast, the compound showed no inhibition of pyruvate kinase, pyruvate, inorg. phosphate dikinase, phosphoenolpyruvate carboxykinase, or enolase, but was an effective inhibitor of phosphoenolpyruvate carboxylase from several C4 and C3 plant species. Of a range of phosphoenolpyruvate analogs reported as inhibitors, I is the only one which shows high selectivity towards phosphoenolpyruvate carboxylase among phosphoenolpyruvate-dependent enzymes.
 IT 108793-81-3F
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphoenolpyruvate carboxylase inhibition by)
 RN 108793-81-3 HCAPLUS
 CN 2-Propenoic acid, 3,3-dichloro-2-[(phosphonooxy)methyl]- (CA INDEX NAME)

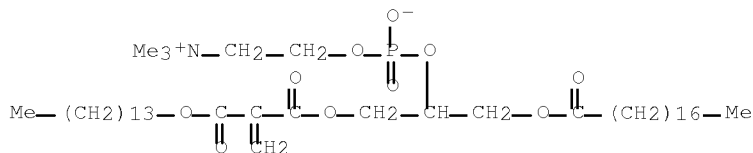


CC 7-3 (Enzymes)
 IT 108793-81-3F
 RL: SPN (Synthetic preparation); PREP (Preparation)
 (preparation and phosphoenolpyruvate carboxylase inhibition by)

L50 ANSWER 11 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1986:403039 HCAPLUS Full-text
 DOCUMENT NUMBER: 105:3039
 ORIGINAL REFERENCE NO.: 105:591a,594a
 TITLE: Polymerizable phospholipids and their polymeric liposomes
 AUTHOR(S): Takane, Minoru; Shigehara, Kiyotaka; Tsuchida, Eishun
 CORPORATE SOURCE: Dep. Polym. Chem., Waseda Univ., Tokyo, 160, Japan
 SOURCE: Makromolekulare Chemie (1986),
 187(4), 853-62
 CODEN: MACEAK; ISSN: 0025-116X
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 13 Jul 1986
 AB Phospholipids containing polymerizable itaconate moieties were synthesized and their formation of liposomes was studied. Although the itaconate phospholipids alone form rather unstable liposomes by ultrasonication, mixts. with other phospholipids such as dipalmitoyl phosphatidylcholine, bis(2,4-octadienoyl) phosphatidylcholine or cholesterol, form stable and single-wall, small sized liposomes. The polymerizability of itaconate phospholipids and the stabilization of such mixed liposomes are discussed.
 IT 102610-88-8F
 RL: PREP (Preparation)
 (preparation of, for liposomes)
 RN 102610-88-8 HCAPLUS
 CN 3,5,8,12-Tetraoxa-4-phosphahexacosan-1-aminium, 4-hydroxy-N,N,N-trimethyl-10-methylene-9,11-dioxo-6-[[[(1-oxooctadecyl)oxy)methyl]-, inner salt, 4-oxide, homopolymer (9CI) (CA INDEX NAME)

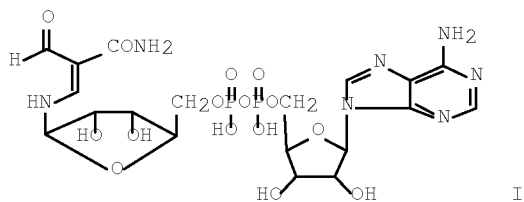
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CRN 102610-87-7
 CMF C44 H84 N O10 P



CC 9-10 (Biochemical Methods)
 Section cross-reference(s): 23, 27
 IT 102583-28-8P 102583-30-2P 102583-32-4P 102610-88-8P
 RL: PREP (Preparation)
 (preparation of, for liposomes)

L50 ANSWER 12 OF 12 HCAPLUS COPYRIGHT 2009 ACS on STN
 ACCESSION NUMBER: 1980:176403 HCAPLUS Full-text
 DOCUMENT NUMBER: 92:176403
 ORIGINAL REFERENCE NO.: 92:28519a,28522a
 TITLE: The peroxidatic reaction catalyzed by horse
 liver alcohol dehydrogenase. 3. Nuclear
 magnetic resonance spectroscopic study of NADX
 AUTHOR(S): Mazzini, Alberto; Dradi, Emanuele; Favilla,
 Roberto; Fava, Adriano; Cavatorta, Paolo;
 Abdallah, Mohamed A.
 CORPORATE SOURCE: Unita Biofis. Mol., Univ. Parma, Parma,
 I-43100, Italy
 SOURCE: European Journal of Biochemistry (1980
), 104(1), 229-35
 CODEN: EJBCAI; ISSN: 0014-2956
 DOCUMENT TYPE: Journal
 LANGUAGE: English
 ED Entered STN: 12 May 1984
 GI

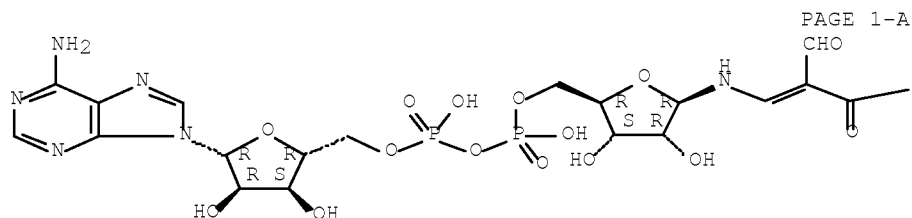


AB As previously reported, horse liver alc. dehydrogenase catalyzes a reaction between NAD and H2O2. The final isolated product is called NADX because of its unknown structure. The results of spectroscopic investigations on this compound are described. They indicated that only the nicotinamide moiety of the original NAD mol. was modified by the action of H2O2. From the 1H and 13C NMR spectra of NADX, the structure I was deduced. This structure was consistent with both UV and reactivity measurements performed on NADX. A tentative mechanism for the whole peroxidatic reaction pathway leading to NADX was proposed.
 IT 73435-45-7
 RL: BIOL (Biological study)
 (enzymic formation and structure of)

10/596,747-301496-EIC SEARCH

RN 73435-45-7 HCAPLUS
 CN Adenosine 5'-(trihydrogen diphosphate), P'→5'-ester with
 2-formyl-3-(β-D-ribofuranosylamino)-2-propenamide (9CI) (CA
 INDEX NAME)

Absolute stereochemistry.
 Double bond geometry unknown.



PAGE 1-B



CC 7-3 (Enzymes)
 IT 73435-45-7
 RL: BIOL (Biological study)
 (enzymic formation and structure of)

10/596,747-301496-EIC SEARCH

FULL SEARCH HISTORY

=> d his nofile

(FILE 'HOME' ENTERED AT 09:02:06 ON 13 JUL 2009)

FILE 'HCAPLUS' ENTERED AT 09:02:25 ON 13 JUL 2009

E US20070293642/PN

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D ALL
D SCA
SEL RN

FILE 'REGISTRY' ENTERED AT 09:04:10 ON 13 JUL 2009

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6/BI OR 107-21-1/BI OR 112-47-0/BI OR 17435-77-7/BI OR
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752235-00-0/BI OR 855894-56-3/BI OR 855894-57-4/BI OR
855894-58-5/BI)
D SCA

L3 6 SEA SPE=ON ABB=ON PLU=ON L2 AND P/ELS
D SCA

FILE 'STNGUIDE' ENTERED AT 09:12:00 ON 13 JUL 2009

D SAV

FILE 'REGISTRY' ENTERED AT 09:12:54 ON 13 JUL 2009

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D SCA
D RN

FILE 'LREGISTRY' ENTERED AT 09:13:42 ON 13 JUL 2009

L5 STR
L6 STR

FILE 'REGISTRY' ENTERED AT 09:55:13 ON 13 JUL 2009

L7 0 SEA SSS SAM L5 AND L6
D QUE STAT

FILE 'LREGISTRY' ENTERED AT 09:55:59 ON 13 JUL 2009

L8 STR L6

FILE 'REGISTRY' ENTERED AT 09:57:05 ON 13 JUL 2009

L9 0 SEA SSS SAM L5 AND L8

FILE 'LREGISTRY' ENTERED AT 10:00:18 ON 13 JUL 2009

L10 STR L8

FILE 'REGISTRY' ENTERED AT 10:04:54 ON 13 JUL 2009

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L12 50 SEA SSS SAM L5
L13 36 SEA SSS SAM L8
L14 50 SEA SSS SAM L5
L15 257255 SEA SSS FUL L5
L16 5 SEA SPE=ON ABB=ON PLU=ON L2 AND L15
L17 0 SEA SUB=L15 SSS SAM L8 AND L5
L18 0 SEA SUB=L15 SSS SAM L8
D QUE STAT

FILE 'LREGISTRY' ENTERED AT 10:56:10 ON 13 JUL 2009

L19 STR L8

FILE 'REGISTRY' ENTERED AT 10:56:54 ON 13 JUL 2009

L20 1 SEA SUB=L15 SSS SAM L19
D SCA
L21 1 SEA SUB=L15 SSS SAM L5 AND L19

10/596,747-301496-EIC SEARCH

D SCA
 L22 30 SEA SUB=L15 SSS FUL L5 AND L19
 D SCA
 L23 0 SEA SUB=L15 SSS SAM L5 AND L8
 L24 18 SEA SUB=L15 SSS FUL L5 AND L8
 SAV TEMP L22 SAS747REG/A
 SAV TEMP L24 SAS747REGA/A
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 C4C8O
 L26 6 SEA SPE=ON ABB=ON PLU=ON L24 AND L25
 D SCA
 E OXIRANE/CN
 L27 1 SEA SPE=ON ABB=ON PLU=ON OXIRANE/CN
 D
 L28 2 SEA SPE=ON ABB=ON PLU=ON L24 AND 75-21-8/CRN
 D SCA
 E METHYLOXIRANE/CN
 L29 1 SEA SPE=ON ABB=ON PLU=ON METHYLOXIRANE/CN
 D SCA
 D
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FILE 'LREGISTRY' ENTERED AT 11:13:38 ON 13 JUL 2009

L33 STR
 L34 STR L33

FILE 'REGISTRY' ENTERED AT 11:15:37 ON 13 JUL 2009

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 D RSD
 E 553.3/RID
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 D SCA
 D SCA L24
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 OR L32) OR L39
 D SCA
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 L43 30 SEA SPE=ON ABB=ON PLU=ON L22 OR L24

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 D QUE STAT L47
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 L49 1 SEA SPE=ON ABB=ON PLU=ON L48 AND L47
 D SCA
 L50 12 SEA SPE=ON ABB=ON PLU=ON L49 OR L47
 SAV TEMP L50 SAS747HCP/A
 D QUE STAT L50
 D L50 1-12 IBIB ED ABS HITSTR HITIND